

Introduction to Swirles

and Intel GPUs in general

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What is Swirles?

- Swirles is our new HPC cluster and the successor to Fawcett.
- There are several partitions (use `sinfo` to check):
 - The Intel components are named Cosmos XI
 - pvc: 3 nodes of Intel Data Center GPU Max 1550 (PVCs), Sapphire Rapids host with 1TB mem.
 - spr: 4 nodes of Sapphire Rapids HBMs
 - ampere: 3 nodes of Nvidia A100, host has 2TB mem
 - lovelace: 1 node of Nvidia L40
 - genoa: 6 nodes of AMD EPYC 9654, 1.5 TB mem
- Intel parts funded by ExCALIBUR as a GPU testbed (open to all UK researchers)
- For now, we haven't worked out a fair usage policy, expect this to change in the future



Access to Swirles

- Two ways to log in:
 1. ssh username@ssh.maths.cam.ac.uk and then use Slurm to queue a job or ssh into a compute node
 2. In your .ssh/config file, define a new entry:

```
Host swirles.maths.cam.ac.uk
User <username>
ProxyJump
username@ssh.maths.cam.ac.uk
IdentityFile ~/.ssh/privatekey
```
- Your username is your CRSid, the password is your usual Maths password for logging into your desktop or Fawcett
- How to check if you have a login (and how long your account is valid for):
<https://useradmin.maths.cam.ac.uk/selfservice/record>
- If you don't have a login, you need to contact Maths IT with a support request: help@maths.cam.ac.uk
- We are in early access mode so it is very possible that IT support cannot fulfill your request without explicit approval from your PhD advisor/line manager.

Slurm on Swirles

How to submit jobs

- You can use mpirun directly from the node (for now...) or you can use Slurm to queue a job (recommended)
- Example Slurm script (also on the GitHub repo):

```
#!/bin/bash

#SBATCH --partition <name>           #<name> can be either pvc, ampere, genoa, spr
#SBATCH --nodes=<#nodes>             #how many nodes
#SBATCH --ntasks=<#tasks>            #how many tasks (MPI ranks) in total
#SBATCH --cpus-per-task=<#cpus>      #set to > 1 to use OpenMP threads
#SBATCH --time=<hh:mm:ss>
#SBATCH --gres=gpu:<#gpus>           #necessary for GPU resources, choose from 1 - 4

export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

cd ${MY_WORK_DIR}
source my_modules.sh

mpirun -np $SLURM_NTASKS ./my_exec
```

Slurm on Swirles

How to submit jobs

- Can also use 'srun' or 'salloc'
- For example:
 - `srun -p pvc --nodes=1 --mpi=pmi2 --cpus-per-task=28 --gres=gpu:1 -
-time=00:30:00 <my_program>`
 - Run my_program on a compute node for 30 min but output to my current terminal
 - `salloc -p pvc --nodes=1 --cpus-per-task=28 --time=00:30:00`
 - Run an interactive job for 30 mins (need to ssh into the compute node yourself)
 - If using mpirun directly on PVCs, use the option `--bootstrap=fork` (this will expose the tiles as separate devices).

The Swirles environment

- Swirles uses a module system, like on Fawcett.
- No modules are loaded by default (try doing a module list)
- To gain access to the modules compiled for Swirles type:
 - `module use /cephfs/software/spack/spack-modules/maths-2024.1/linux-ubuntu22.04-x86_64_v4`
 - Some essential modules:
 - `module load cmake`
 - `module load miniforge3/4.8.3-4-Linux-x86_64/gcc/s2ikv54u`
 - `module load python/3.11.7/gcc/swa4n3ak`
 - Then use a virtual env to install the python packages that you need.
- The OS is Ubuntu 22.04
- Editors are vi or nano - But I have an emacs installation which you are welcome to use:

```
/alt/applic/user-maint/jk945/emacs
```

Just make an `alias` or add it to your `PATH` in `.bashrc`

Compilers on Swirles

- For an Intel oneAPI environment:
 - `module load intel/compiler-intel-llvm/2024.2.0`
 - `module load intel/mpi/2021.13`
 - `module load intel/mkl/2024.2`
 - The MPI compiler is then `mpiicc/mpiicpx/mpiifx`
- For a GNU environment:
 - `module load gcc`
 - `module load openmpi`
 - The MPI compiler is then `mpicc/mpicxx/mpif90`
- For CUDA:
 - `module load cuda/12.6.3/gcc/bxp4amlg`
 - The compiler is `nvcc`
 - There is no CUDA enabled MPI library yet
- NB: You can type `'which mpirun'` to check your version of MPI

Example environment setup

On the sw-pvc0X nodes, type: `source /local/scratch/public/swirles-env.sh` to set up the following environment

```
#!/bin/bash

module load intel/compiler-intel-llvm/2024.2.0
module load intel/mpi/2021.13
module load intel/mkl/2024.2

export I_MPI_PMI_LIBRARY=/usr/lib/x86_64-linux-gnu/libpmi2.so #this points Slurm to the API (PMI-2) for launching MPI jobs
export I_MPI_OFFLOAD=1 #this allows GPU to GPU direct communication via MPI (GPU aware MPI)
unset ZE_AFFINITY_MASK #if this is set, then GPU pinning is automatically disabled
export ZE_FLAT_DEVICE_HIERARCHY=FLAT #exposes tiles as separate devices
export I_MPI_OFFLOAD_TOPOLIB=level_zero #set interface for GPU topology recognition to level zero
export I_MPI_OFFLOAD_PIN=1 #enable GPU pinning (somewhat degenerate with I_MPI_OFFLOAD)
export I_MPI_DEBUG=3 #this prints pinning information

alias my_sysmon='watch -n 1 /alt/applic/user-maint/jk945/pti-gpu/tools/sysmon/install/bin/sysmon'
```

This contains all the environment variables you need to run a SYCL program or use MPI enabled GPU communications or use Slurm with multiple GPUs per job

More info at Miren's guide to running GRTeclyn on Dawn: <https://github.com/GRTLCollaboration/GRTeclyn/issues/67>

Storage on Swirles

Where do I put my stuff?

- /home/<username> should be the same as on Fawcett/local desktop
- You should have space for outputs on /cephfs/store/<group-name> - the amount of space each group has depends on their level of contribution towards the purchase of the system.
- There is an additional 5 GB for user wide installations of software at /alt/applic/user-maint/<username>

Hands-on demos

- There are some simple MPI, SYCL, Pytorch scripts in the GitHub repo
 - Load your preferred modules (this must be the Intel oneAPI libraries if using SYCL)
 - Compile: `mpicpx -c test_sycl.cxx`
 - Link: `mpicpx -o test_sycl.out -fsycl test_sycl.o`
- Try out your own codes:
 - Pluto: OK
 - Athena++: OK
 - Idefix: Limited functionality, Serial host + CUDA: OK, MPI + OpenMP: OK, MPI + CUDA: Not currently possible, MPI+SYCL: Not currently possible